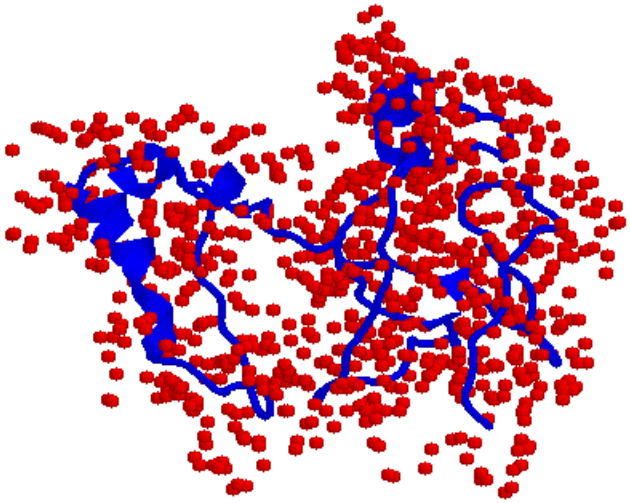
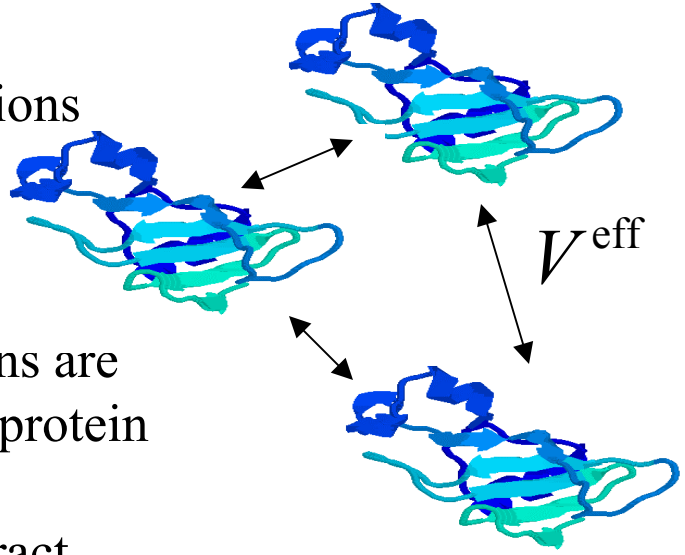
Coarse-Grained Simulation Methods for Complex Fluids: Venkat Ganesan: DMR 0204199

Recent advances in nanotechnology and synthetic chemistry have brought to fore significant challenges to our understanding and the prediction of the thermodynamics and dynamics of systems containing *many components, typically with disparate size and time scales*. Research in our group focuses on addressing these challenges by developing coarse-grained computer simulation methods to address phenomena on experimentally relevant length and time scales. For instance, the effect of solvent molecules (denoted by red spheres on the first figure) on the phase behavior of protein solutions is addressed by the development of "implicit solvent' models which coarse-grains the solvent molecules to describe the interactions between the proteins by effective potentials. Simulations using such interactions are used to shed light on the fundamental mechanisms of protein crystallization --- a technologically important phenomena in addition to its role in diseases like cataract.





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Education:

1 Graduate student (Ms. Surve) and 1 Postdoctoral associate (Dr. Pryamitsyn) are currently working on different aspects of this project. As a part of their education, both of them attended the American Physical Society's Annual Meetings and the Gordon Research Conference in Polymers. Dr. Pryamitsyn also presented his research in both settings.

An Undergraduate student (Mr. Shayib) in his junior year has recently joined our group. He is being mentored by Ms. Surve and is expected to pursue graduate education upon completion of his BS degree.

Outreach:

We have recently become involved with the Office of Equal Opportunity in Engineering (a program aimed at increasing the minority representation in Engineering) at Austin to explore if some of our simulation modules can be modified to be used in their outreach programs.

We have also become recently involved with the RPI's initiative Virtual Polymer Laboratory (http://block.chem.rpi.edu/html/E_Outreach/) , targeting high school science teachers, to incorporate some simple simulation modules that can be used to demonstrate molecular concepts of polymer physics to high school students.